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A simple particle pack generation method with predefined grain size distribution and porosity using the discrete element method

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Abstract. In numerical studies of granular materials, it is often important to realize simulations considering the realistic granulometry of a sample of the material. In case of soils, in particular, grain size distribution could greatly influence the material´s behavior. The aim of this work is to present a simple and rapid method for generating particle packs with predefined grain size distribution and porosity for discrete element simulations. It is a dynamic algorithm with simple input data. The methodology considers spherical particles only. The particles' radii are determined during the generation process based on the percent fraction of total particles passing thru a sieve and the sieve mesh size, according to a given granulometric curve and sample porosity, mimicking a real granulometric characterization in laboratory. Differently from existing methodologies, the particles are generated until the desired retained mass in each sieve is reached. The generated particles are positioned randomly within a pre-defined domain in a non-contacting way using a random sequence addition (RSA) algorithm, and then are submitted to "jamming" pseudo forces. The method proved very effective and showed good results (in terms of attained grain size distribution and porosity) as illustrated in numerical examples.

Keywords: Particle pack generation, Grain size distribution, Discrete element method.

1 Introduction

Before carrying out a simulation of granular materials through discrete element analysis, one has always to generate a particle pack or a sample of particles. It is possible to generate samples either using the discrete element method (DEM) itself or not. Available generation methodologies are typically sorted as dynamic or of geometric build. The dynamic methodology involves the use of the DEM itself as to achieve denser samples – although much more time for the generation is needed. The geometric method, in turn, proposes to occupy the domain with particles calculating their positions through pure geometric arguments, and without changing the position vector of each particle over the generation process (BAGI [1]). It is well-known that the mechanical behavior of a sample of granular material may be quite complex, especially at the mesoscale. To achieve a realistic numerical simulation, the sample generation has not only to fill up the proposed domain but also to build a sample with the correct mass density and porosity, while at the same time having the particles as close as possible to the material´s real size distribution. We recall that the material's behavior could be greatly influenced by the grain size distribution. The consideration of the particle size distribution is thereby critical for DEM simulations.

Dang and Meguid [2] was one of the first attempts to consider the grain size distribution in the particle generation method. In their method, the domain is divided into a finite number of equally smaller samples. Then the particles are generated inside one of the smaller samples. Their radii are calculated with parameters provided by a given gradation test. The particle generation will stop when the total volume of the (smaller) sample is reached. After this step, the sample is compressed and shaked. The second step is the replication of this smaller sample as to fill up the original domain´s dimensions, thus maintaining the gradation distribution and porosity of the smaller

sample. Although certainly an advance, the proposed methodology proved not able to accurately replicate certain granulometric distributions.

The present work develops a simple methodology with consideration of the gradation distribution curve and imposed porosity, based on the particle radius technique from Dang and Meguid [2] (with origin in Fu and Dekelbab [3]), however using the retained mass in the smaller nominal mesh of a pair of sieves from a given granulometric curve as the limitational parameter for generating new particles. This modification in Dang and Meguid´s original methodology proved to allow samples with the correct granulometric distributions for different types of gradation curves, such as (but not only) well-graded and gap-graded. This is illustrated in numerical examples. The paper is organized as follows. In Section 2 we present our technique. In Section 3 we use the technique to generate packs with predefined grain size distributions and porosity, and compare the outcomes against Dang and Meguid´s [2] and other existing methods. In Section 4 we close this paper with our conclusions and final considerations. Throughout the text, plain italic letters $\left(a,b,\ldots,\alpha,\beta,\ldots,A,B,\ldots\right)$ denote scalar quantities.

2 The proposed technique

Our technique creates a layer (or layers upon layers) of particles inside a predefined domain or recipient, with given porosity and the particle sizes following an input gradation curve. The method applies random sequence addition, followed by a "jamming" process until a desired total height for the sample is reached. The process is extremely simple as it will be presented below. It is schematically illustrated in Figure 1.

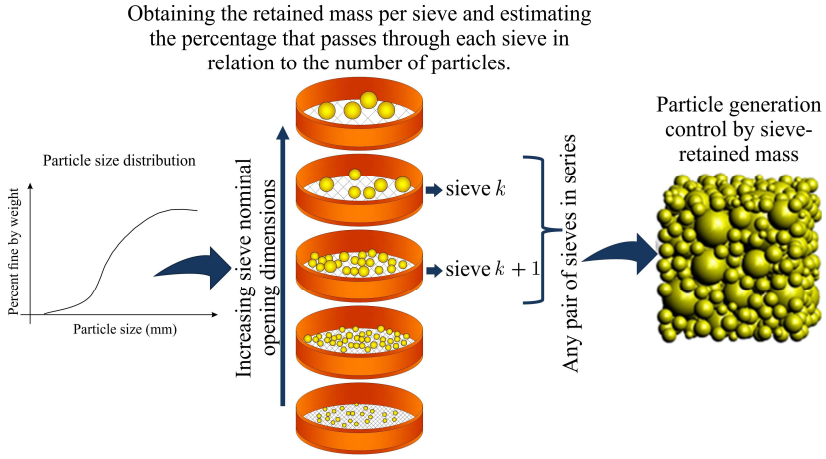


Figure 1. Scheme of the proposed methodology: input (given) gradation distribution, sieving characterization and generated particle sample

The particles´ shape is restricted to spheres in this work. The method starts by setting the geometry parameters (shape and dimensions) of the domain that will contain the sample. For the sake of simplicity (but without any loss of generality), we will consider only prismatic domains here. Let us denote the domain´s interior volume by V, and the sample´s desired porosity (ratio of the void´s volume to total volume) by n. The total volume of particles to be generated, V_p, is given by

$$V_p = V \times \left(1 - n\right). \tag{1}$$

Defining ρ_p as the specific mass of the particles´ constituent material, the total mass of particles m_p to be generated may be written as $\rho_p \times V_p$.

In case the sample is subjected to a sieving characterization test, this total mass would be partially retained in each of the sieves that make up the series of N_S sieves. The percentage of mass $\%Q_m^k$ that would pass through each sieve k, $k = 1,2,\ldots,N_S$, may be determined from the given (input) gradation curve. Assuming that the sieves are numbered consecutively from the largest to the smallest mesh opening (see Figure 1), it is possible to compute the retained mass in each sieve, $m_p^{ret,k}$, through the following expression

$$m_p^{ret,k} = \left(\%Q_m^k - \%Q_m^{k-1}\right) m_p \,. \tag{2}$$

Considering this retained mass in each sieve and the volume of a standard particle defined for each pair of sieves, V_p^{standard}, it is possible to estimate the number of the retained particles in the smaller mesh opening of the pair, $N_p^{ret,k}$ as follows

$$N_p^{ret,k} = \frac{m_p^{ret,k} \Big/ \rho_p}{V_p^{\text{standard}}}\,, \tag{3}$$

where we define the diameter of the standard particle for the pair as the average between the openings of the meshes of the corresponding sieves, k and $k+1$. So, the percentage of number of particles $\%Q_p^k$ that would pass through each sieve is given through

$$\%Q_p^k = \left(\frac{N_p - N_p^{ret,k,acc}}{N_p}\right) \times 100\,, \tag{4}$$

where N_p is the total number of particles of the sample and $N_p^{ret,k,acc}$ is the accumulated number of retained particles in each sieve k.

The input parameters of the generation method are: (i) the number of sieves in the series and their respective mesh sizes or openings (which, as said above, correspond to the diameter of the smallest particle that can be retained in each sieve), taken from the given gradation curve; (ii) the retained mass in each sieve, as computed from eq. (2); and (iii) the passing percentage through each sieve in terms of number of particles, as computed from eq. (4). We generate the particles by looping over the pairs of sieves in the series, from the largest to the smallest (we remind that k is the sieve with larger opening of the pair and $k+1$ the immediate smaller one, as shown in Figure 1), and such that each newly created particle has its diameter randomly determined in between the openings of the two sieves of the corresponding pair in the loop. This is done according to the following expression, which is based on Dang and Meguid [2]:

$$r_i = \frac{1}{2}\Big[\, D_{k+1} + \left(Random - \%Q_p^{k+1}\right) \times \left(D_k - D_{k+1}\right) / \left(\%Q_p^k - \%Q_p^{k+1}\right)\Big], \tag{5}$$

where r_i is the radius of the newly created particle i, D_k and D_{k+1} are the diameters (or mesh openings) of the pair of sieves to which particle i "belongs" or is retained in between (with $D_k > D_{k+1}$), $\%Q_p^k$ and $\%Q_p^{k+1}$ are the passing percentages (in terms of number of particles) for the two sieves of the pair, and $Random$ is a randomly generated number, where $\%Q_p^{k+1} < Random < \%Q_p^k$. For each pair of sieves in the loop, the particle creation occurs until the total mass of particles with this diameter range reaches the retained mass in the sieve of smaller nominal mesh size $k+1$ of the pair. The retained mass in each sieve is given by eq. (2) and must be computed for all sieves of the series prior to the beginning of the loop. We recall that this data is one of the input parameters for the algorithm. It is important to remark that the method proposed by Dang and Meguid [2] does not follow such mass control approach, but instead tracks the number of particles in each pair of sieves and controls the total volume of particles, which ultimately (and of course) deviates from the desired gradation curve and the desired porosity. By doing this slight change in the generation control, we are able to generate packs that very accurately reproduce the input gradation curve as well as the input sample´s porosity, as it will be shown in the next section.

As proposed by Campello and Cassares [4], each generated particle has its position within the domain attributed randomly using simple random sequence addition (RSA) techniques (see, e.g., Torquato and Stillinger [5]). This is done in a non-overlapping way, meaning that if a particle is attributed a position such that it overlaps with previously generated particles, it is discarded, and a new particle is created. This requires a contact detection scheme, which in this case is very simple since we are dealing with spherical particles here. Once the generation is completed, the particles are set to deposit at the bottom of the domain by gravitational settling, and this is done through a DEM simulation. The result is a rather compact pack of particles, mimicking a real sample of granular material. We recall that the generation can be done either in a single layer or in a layer-wise way. In the latter case, the generation is done in steps, with each step corresponding to the generation of a new layer of thickness h_0 (see Fig. 2). The process is then repeated until the predefined domain height H_d is achieved ^{h_d}. We refer the interested reader to Campello e Cassares [4] for details.

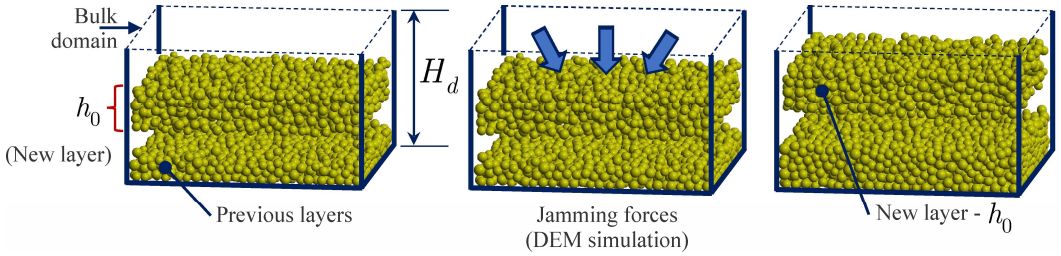


Figure 2. Schematic illustration about the packing procedure. Deposition is done through gravitational settling.

It is important to highlight that this methodology does not resort to radius increase during the deposition stage. Together with the consideration of a given gradation curve, this is a marked difference between our technique and the widely used method by Lubachevsky and Stillinger [6], and its several variations. As a result, our algorithm fully replicates the predefined gradation distribution.

Regarding the deposition stage, the main aspects to be controlled to achieve a nicely compact sample with computational efficiency are: (i) selection of appropriate elastic parameters for the particles (this will govern the time-step size of the simulation); (ii) the use of an explicit instead of implicit time integration scheme within the DEM; (iii) the initial volume fraction of particles must be set to around $\phi_0 \approx 0.4$ for 2D packs and to $\phi_0 \approx 0.25$ for 3D packs; (iv) consideration of rotational motion of the particles and appropriate inter-particle friction.

It's important to highlight that for Fu and Dekelbab [3] and Dang and Meguid [2], the particle generation is stopped when the total volume of particles is achieved. In our methodology, in contrast, we use the retained mass in each sieve as the control parameter. This consideration allows a remarkably better adherence to the desired gradation distribution curve, as it will be seen below. It is worth noting that Dang and Meguid [3] defined the total solid volume as the result of the multiplication of the porosity with the sample´s domain volume. Here, instead, we are not applying this consideration, since we find it inconsistent with the very definition of porosity. We employ eq. (1) instead.

3 Examples

In this section, a few examples are showed to verify the proposed methodology and its effectiveness. After the particle generation, the deposition stage is done by gravitational settling. This phase is numerically solved via the discrete element method considering a soft-sphere approach. During the calculation of the interactions between particles, we consider gravity forces, contact forces (through Hertz's contact theory), friction forces (through Mindlin's theory with stick-slip) and rolling resistance effects. The interested reader is referred to Campello [7]-[8], Campello and Zohdi [9], Wellmann and Wriggers [10], and Zohdi [11]. For time integration, we adopt an explicit (forward Euler) scheme because contacts and collisions have typically a very short duration, thereby requiring very small time-steps for an accurate integration of the contact forces (see Campello [8]). We determine the duration of a typical contact or collision Δt_{con} by

$$\Delta t_{con} \cong 2.87 \left[\frac{(m^*)^2}{r^* (E^*)^2 v_{rel}} \right]^{\frac{1}{5}}, \tag{6}$$

where v_{rel} is the relative velocity of a typical contacting pair in the pair's central direction immediately before the contact or collision is initiated. The time-step size is taken as a tenth of the duration of a typical contact. The results obtained here for each example using the proposed method are compared with results obtained by Dang and Meguid [2] (for the first example), commercial licensed software PFC3D 7.00 of Itasca Consulting Group, Inc. [12] and Rocky DEM of ESSS Company [13]. It is important to highlight that the same amount of information regarding each granulometric curve is used for all applied methods in this work and we chose to present the graphs with arithmetic instead of logarithmic scale for better visualization of results.

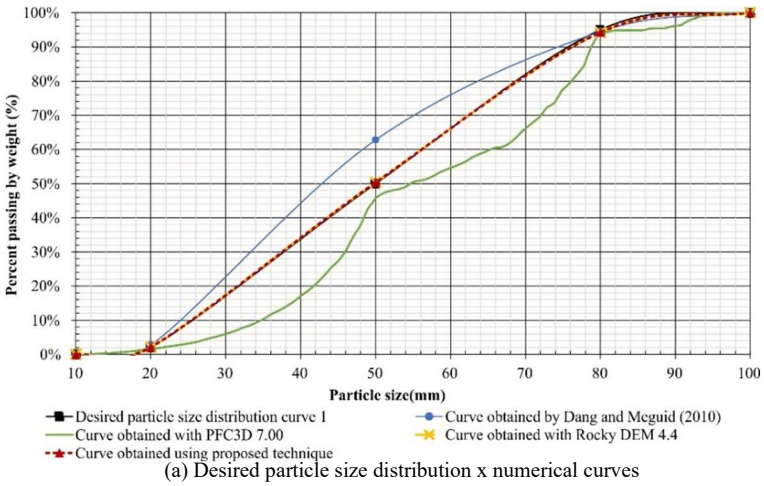
3.1 Sample from Dang and Meguid [2]

A sample was generated considering a gradation distribution curve proposed by Dang and Meguid [2]. The data used by Dang and Meguid [2] is shown in Table 1. The domain for generating the sample and validating the algorithm consists of a cube with dimensions of 0.50 m x 0.50 m x 0.50 m. We consider a specific mass of 2600 kg/m³ and a porosity of 0.38, as provided by Dang and Meguid [2]. The other data are as follows: elastic properties of the particles: $E_i = 1.5 \times 10^7$ Pa and $\nu_i = 0.50$; friction coefficients between particles and particle-walls: 0.30; contact, friction and rolling damping rates: 0.20; rolling resistance coefficient: 0.20; gravity acceleration: 9.81 m/s² (y-direction); time-step size: $1x10^{-5}$ s.

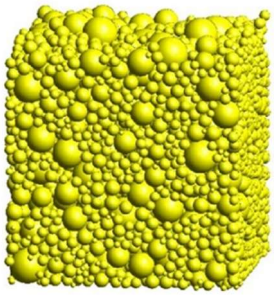
Table 1. Desired particle size distribution for example 3.1: input data and obtained results (percent errors in parentheses)

Particle size mm	% passing (number of particles)	Percent passing by weight				
		Desired curve 1	Dang and Meguid [2]	Proposed technique	PFC3D 7.00 [12]	Rocky DEM 4.4 [13]
100	100.0%	100.0%	100.00% (0.00%)	100.00% (0.00%)	100.00% (0.00%)	100.00% (0.00%)
80	99.61%	95.0%	94.46% (-0.57%)	94.41% (-0.62%)	93.90% (-1.16%)	94.25% (-0.78%)
50	90.90%	50.0%	62.77% (25.54%)	49.66% (-0.68%)	45.63% (-8.73%)	50.35% (0.71%)
20	31.47%	2.0%	2.72% (36.00%)	1.99% (-0.69%)	1.63% (-18.25%)	2.10% (5.19%)
10	0.0%	0.0%	0.00% (0.00%)	0.00% (0.00%)	0.00% (0.00%)	0.00% (0.00%)

Figure 3(a) shows the desired curve and the curves obtained for this sample. It is possible to observe that there is a great adherence between the desired curve and the curve obtained with our method. This observation can also be made when analyzing the relative percentage errors evaluated between the data from the target curve and the numeric results from the proposed method (see errors in parentheses in Table 1). It is important to highlight that the relative percentage errors observed for the methodology proposed by Dang and Meguid [2] are between 25% and 36%, whereas for our method the maximum is 0.69%. The performance obtained using PFC3D was not satisfactory, as compared to that from Rocky DEM and our method. This indicates that the particle generation based on the total volume of particles is not able to achieve good results in all points of the curve. The curve obtained with Rocky DEM software, in turn, can be considered with good adherence to the desired curve. Despite the good results, the curve that comes closest to the desired curve is the one obtained with our method. Regarding the attained porosity, we obtained 0.388, which is pretty close to the desired value. Dang and Meguid [2] obtained a sample with porosity of 0.379, and the Rocky DEM a porosity of 0.368. We note that it was not possible to compute the porosity for the sample generated with PFC3D. Figure 3(b) shows the sample obtained using the herein proposed method.



(a) Desired particle size distribution x numerical curves



(b) Sample generated according to granulometric curve after deposition step (5,649 spheres)

Figure 3. Particle size distributions for example 3.1 – (a) desired and numerical curves and (b) sample obtained with our method

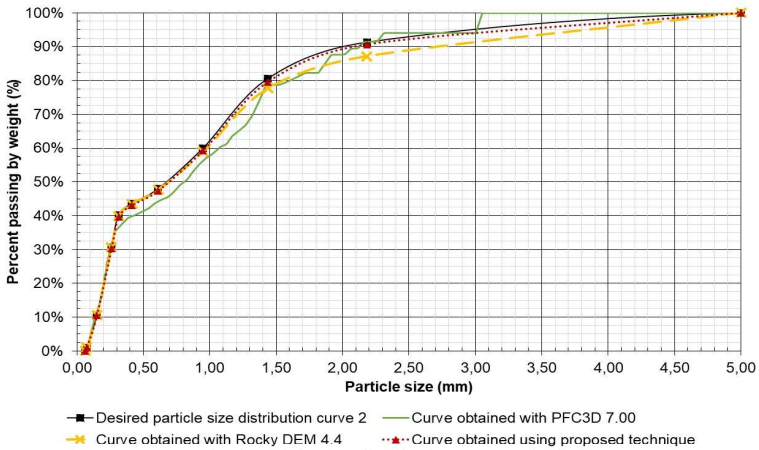
3.2 Gap-graded sand sample

This is a gap-graded sample with properties taken from Pinto [14]. The input data are a specific mass of 2600 kg/m³, a porosity of 0.38 and the gradation curve shown in Table 2. Dimensions for the domain of the sample are 0.010 m by 0.010 m (base) and 0.005 m (height). These data lead to a sample with spheres of radius between 0.057 mm and 5 mm and a total of nearly 85000 particles. The other data are as follows: elastic properties of the particles: $E_i = 2.7 \times 10^7$ Pa and $\nu_i = 0.25$; friction coefficients between particles and particle-walls: 0.25; contact, friction and rolling damping rates: 0.90; rolling resistance coefficient: 0.30; gravity acceleration: -9.81 m/s² (y-direction); time-step size: 1×10^{-7} s.

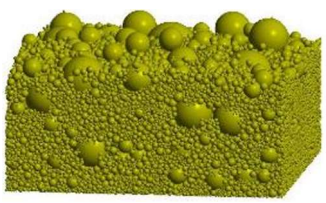
Table 2. Desired particle size distribution for example 3.2: input data and obtained results (percent errors in parentheses)

Particle Size mm	Retained mass (kg)	Percent passing (number of particles)	Percent passing by weight			
			Desired curve 2	Proposed Technique	PFC3D 7.00 [12]	Rocky DEM 4.4 [13]
5.000	0.000000000	100.000%	100.0%	100.00% (0.00%)	100.00% (0.00%)	100.00% (0.00%)
2.184	0.000070122	99.999%	91.3%	90.67% (-0.69%)	91.51% (-0.23%)	87.17% (-4.53%)
1.438	0.000086645	99.984%	80.6%	79.58% (-1.21%)	78.65% (2.35%)	77.68% (-3.57%)
0.950	0.000165633	99.889%	60.0%	59.26% (-1.23%)	56.30% (6.17%)	58.93% (-1.78%)
0.612	0.000096720	99.691%	48.0%	47.39% (-1.28%)	44.28% (7.76%)	47.69% (-0.65%)
0.413	0.000035464	99.432%	43.6%	43.04% (-1.29%)	39.85% (8.60%)	43.43% (-0.39%)
0.314	0.000028210	98.857%	40.1%	39.58% (-1.29%)	36.57% (8.79%)	39.95% (-0.37%)
0.260	0.000075764	95.717%	30.7%	30.30% (-1.29%)	31.46% (-2.47%)	30.68% (-0.07%)
0.150	0.000162006	77.291%	10.6%	10.46% (-1.29%)	11.67% (10.07%)	10.67% (0.66%)
0.075	0.000077376	24.042%	1.0%	0.99% (-1.29%)	-	1.01% (0.96%)
0.063	0.000008060	0.000%	0.0%	0.00% (0.00%)	0.00% (0.00%)	0.00% (0.00%)

Results obtained with the proposed method and with other two software are presented in Figure 4(a). Our method achieved very good results when comparing to the input curve from Pinto [14]. The relative percent errors are presented in Table 2 (see values in parentheses). Note that there is a greater difference in the percentage errors of mass that passes through the sieves between the diameters of 0.150 and 1.438 mm for the curve obtained with PFC3D 7.00. In contrast, the curve obtained with our method shows significantly lower relative errors, with values less than 1.3% (in modulus). As for the performance of the Rocky DEM, it did not generate a sample with adherent characteristics for diameters greater than 1.438 mm and 2.184 mm. For particles smaller than 0.950 mm, however, good results are observed. Regarding the porosity, the value obtained with proposed methodology is 0.382 (a difference of only 0.53% to the desired value). For the Rocky DEM sample, the obtained porosity is 0.303, rather different from the desired value (relative error of 20.3%). The sample obtained with our method is shown in Figure 4(b).



(a) Desired particle size distribution x numerical curves



(b) Sample generated according to granulometric curve after deposition step (81,573 spheres)

Figure 4. Particle size distributions for example 3.2 – (a) desired and numerical curves and (b) sample obtained here

4 Conclusions

The main objective of this work was to present a particle sample generation methodology considering an input gradation distribution curve and a predefined porosity for DEM simulations. The method generates particles limited to predefined diameter intervals. The method keeps creating new particles until the particles reach a certain mass, corresponding to the retained mass in sieves of a corresponding gradation characterization in laboratory. This consideration, though sounds rather obvious, was not performed by existing methods and proved to be an adequate improvement. As it has been shown, it was possible to generate samples according to the desired gradation distribution curve. Plus, the porosity obtained is pretty close to the desired value. As a last note, the algorithm is very straightforward to implement and use. We believe it may be very useful for discrete element simulations of soil samples, to which the realistic granulometry is critical.

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